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U.S. Environmental Protection Agency
Chemical Right-To-Know Program
PO Box 1473
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July 8, 2003

Dear Sir/Madam:

Cytec Industries Inc. is responding to the EPA Comments on the robust summaries and test plan for m-diisopropenylbenzene (CAS No. 3748-13-8).

The responses below are in order corresponding to the key issues in the EPA comments.

Physicochemical Properties

The Agency recommends that the water solubility study be rerun following OECD TG 105. The basis for this recommendation is that the estimated and measured values for m-diisopropenylbenzene (CAS No. 3748-13-8) are not close to an EPIWIN experimental value for the water solubility of diisopropylbenzene (CAS No. 25321-09-9). In preparing the test plan Cytec Industries Inc. considered CAS No. 25321-09-9 as a possible data rich surrogate, but rejected it as not being a suitable analog. This decision was made even though use of this analog would offer the opportunity to use surrogate data for some endpoints and would possibly eliminate the need for conducting some mammalian toxicity testing. The submitter believes that the absence of double bonds in the alkyl side chains of diisopropylbenzene can lead to significant differences in properties between diisopropylbenzene and diisopropenylbenzene, the latter having carbon-carbon double bonds in the side chains. Further, CAS No. 25321-09-9 is a mixture of ortho-, meta- and para- isomers, whereas the test substance is the pure meta isomer. A database exists also for CAS No. 99-62-7 (1,3-diisopropylbenzene), which, at least, is also pure meta. This possible analog was also rejected, since it lacks double bonds in the alkyl side chain.

We note that measured and estimated values for water solubility of the test substance are in good agreement, and that the measured value was obtained using a well conducted study. Therefore, we do not see a need to rerun solubility.

Photodegradation

The agency requests that the submitter comment with respect to the potential for the test substance to undergo direct photolysis. As noted in both the robust summary dossier and the test plan, the EPIWIN Aop program predicts that the test substance readily undergoes indirect hydroxyl radical-induced photodegradation in the

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atmosphere. We have not found any information with regard to direct photolysis. Based on the molecular structure, photolysis (direct or hydroxyl radical induced) would be most likely to occur at the side chains, rather than at the benzene ring. Hydroxyl radical-induced photodegradation is likely to occur more quickly and be a more important degradative pathway than direct photolysis. The Hazardous Substance Data Bank Toxnet has a record for divinylbenzene (CAS No. 1321-74-0). This substance has the same functionality as the test substance, the difference in molecular structure being that divinylbenzene has two ethenyl side chains attached to the benzene ring (whereas the test substance has two propenyl side chains attached, i.e., the two compounds are homologs). Toxnet states, "Reactions with photochemically produced hydroxyl radicals (estimated half-life of 7 hr) and ozone (estimated half-life of 6.5 hr) in the atmosphere are likely to be important fate processes." Nothing is said with respect to direct photolysis. This reference lends some support to the suggestion that direct photolysis is a less important degradative pathway in the atmosphere for the test substance.

Guidance for Testing Closed System Intermediates

The EPA has raised some issues with respect to use of m-diisopropenylbenzene as a closed system intermediate. Cytec Industries Inc. has recently learned that there is a minor use of the test substance that may not allow for qualification of the material solely as a closed system intermediate. Therefore, Cytec Industries Inc. is withdrawing its claim for reduced testing and has revised its test plan to address the full battery of SIDS endpoints.

As stated in the revised test plan, Cytec Industries Inc. agrees to conduct the following studies to address identified data gaps:

1. Chromosomal aberration (OECD TG 473)
2. Combined oral reproductive/developmental toxicity screen (OECD TG 421).

Ecological Effects

The Agency suggests that the aquatic study robust summaries be supplemented with QSAR data. Accordingly, the IUCLID dossier has been revised to include the QSAR estimates, which were run using EPIWIN ECOSAR with measured inputs for melting point, boiling point, vapor pressure and water solubility. The test plan has also been revised to show the comparison.

Conclusion

Cytec Industries Inc. appreciates the opportunity to respond to the EPA comments. The robust summary set and test plan have been revised in response to the comments. Testing is planned to address the data needs identified, and on completion of the studies the new data will be summarized and included in the summary set and test plan.

Yours truly,

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